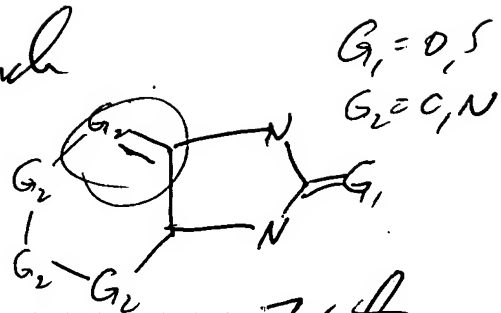
Connecting via Winsock to STN 10/689,924

Welcome to STN International! Enter x:x structure search



LOGINID:SSSPTAAJP1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

7 hits

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	4	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	5	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	6	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	7	MAR 02	GBFULL: New full-text patent database on STN
NEWS	8	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	9	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	10	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	11	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	12	MAR 22	PATDPASPC - New patent database available
NEWS	13	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	14	APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	15	APR 04	EMBASE - Database reloaded and enhanced

NEWS EXPRESS	JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:03:24 ON 06 APR 2005

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:03:33 ON 06 APR 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2005 HIGHEST RN 847968-12-1
DICTIONARY FILE UPDATES: 5 APR 2005 HIGHEST RN 847968-12-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

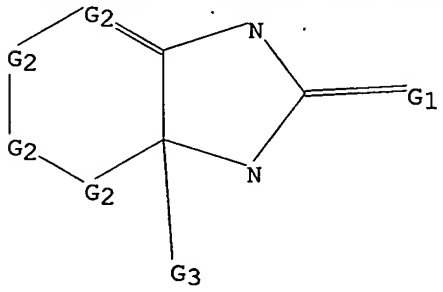
Please note that search-term pricing does apply when conducting SmartSELECT searches.

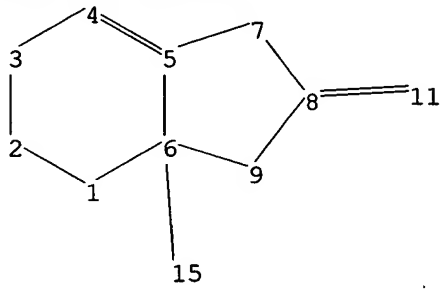
****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10681924h.str





chain nodes :
11 15
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
6-15 8-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 6-15 7-8 8-9 8-11

G1:O,S

G2:C,N

G3:Cy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS
15:CLASS

L1 STRUCTURE UPLOADED

=> s L1
SAMPLE SEARCH INITIATED 15:03:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 11643 TO ITERATE

8.6% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 226395 TO 239325
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s L1 full
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FULL SCREEN SEARCH COMPLETED - 233513 TO ITERATE

100.0% PROCESSED 233513 ITERATIONS 32 ANSWERS
SEARCH TIME: 00.00.06

L3 32 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 161.33 161.54

FILE 'CAPLUS' ENTERED AT 15:04:03 ON 06 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 6 Apr 2005 VOL 142 ISS 15
FILE LAST UPDATED: 5 Apr 2005 (20050405/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s L3

L4 7 L3

=> d 1-7 ibib abs hitstr

L4 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:331928 CAPLUS
DOCUMENT NUMBER: 140:357354
TITLE: A preparation of benzimidazolone derivatives useful as anti-inflammatory agents
INVENTOR(S): Dhar, T. G. Murali; Potin, Dominique; Maillet, Magali Jeannine Blandine; Launay, Michele; Nicolai, Eric Antoine; Iwanovicz, Edwin J.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004032861	A2	20040422	WO 2003-US31960	20031009
WO 2004032861	A3	20040805		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004116467	A1	20040617	US 2003-681924	20031009
PRIORITY APPLN. INFO.:			US 2002-417935P	P 20021011
OTHER SOURCE(S):	MARPAT 140:357354			

GI

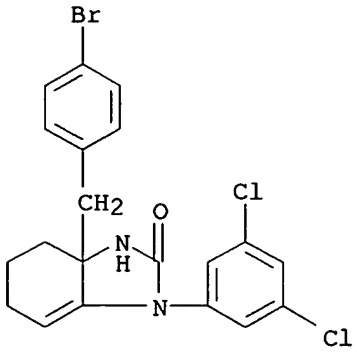
our app.

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

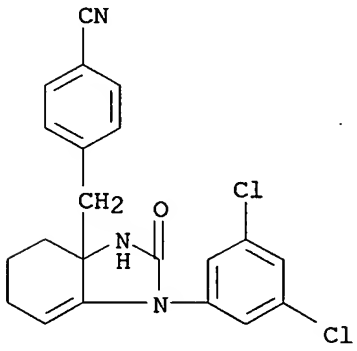
AB The invention relates to benzimidazolone derivs. of formula I [wherein: K is O or S; Q is a bond or C(O), etc.; Ar is (un)substituted (hetero)aryl; J1 is a bond, -N(R4)-, etc.; J2 and J3 are -N(R4)- or (un)substituted CH2, etc.; Y and Z are independently selected from N, (un)substituted CH, etc.; R1 = H, (un)substituted alk(en)yl, (hetero)aryl, cycloalkyl, etc.; R2 and R3 are independently selected from H, halogen, NO2, CN, (un)substituted alk(en)yl, etc.; R4 is H, (un)substituted alk(en)yl, CN, C(O)-alkyl, O-alkyl, etc.], their enantiomers, diastereomers, and pharmaceutically-acceptable salts, useful as anti-inflammatory agents. Compds. I were tested in an H1-HeLa adhesion assay and in a HUVEC (human umbilical vein endothelial cells) adhesion assay (no biol. data). For instance, benzimidazole derivative II was prepared via intramol. heterocyclization of the obtained urea derivative III, and N-acetylation of the obtained benzimidazole derivative IV (no yield data).

IT **681261-14-3P 681261-15-4P 681261-21-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzimidazolone derivs. useful as anti-inflammatory agents)

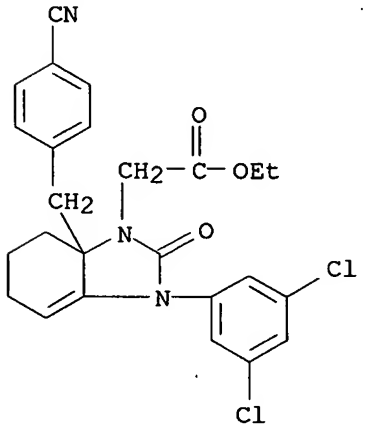
RN 681261-14-3 CAPLUS
CN 2H-Benzimidazol-2-one, 3a-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro- (9CI) (CA INDEX NAME)



RN 681261-15-4 CAPLUS
CN Benzonitrile, 4-[[1-(3,5-dichlorophenyl)-1,2,3,4,5,6-hexahydro-2-oxo-3aH-benzimidazol-3a-yl]methyl]- (9CI) (CA INDEX NAME)



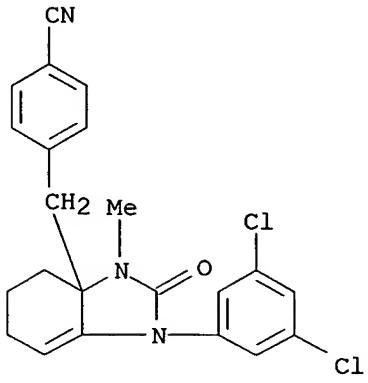
RN 681261-21-2 CAPLUS
CN 1H-Benzimidazole-1-acetic acid, 7a-[(4-cyanophenyl)methyl]-3-(3,5-dichlorophenyl)-2,3,5,6,7,7a-hexahydro-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



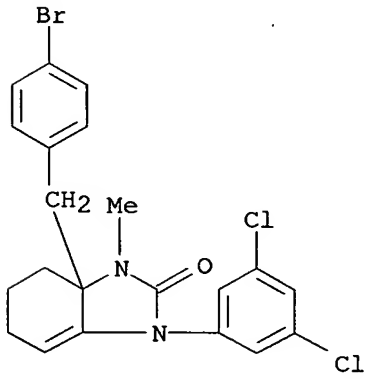
IT **681261-16-5P 681261-17-6P 681261-18-7P**
681261-19-8P 681261-20-1P 681261-22-3P

681261-23-4P 681261-24-5P 681261-25-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzimidazolone derivs. useful as anti-inflammatory agents)

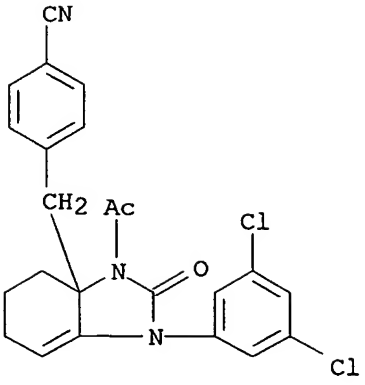
RN 681261-16-5 CAPLUS
CN Benzonitrile, 4-[[1-(3,5-dichlorophenyl)-1,2,3,4,5,6-hexahydro-3-methyl-2-oxo-3aH-benzimidazol-3a-yl]methyl]- (9CI) (CA INDEX NAME)



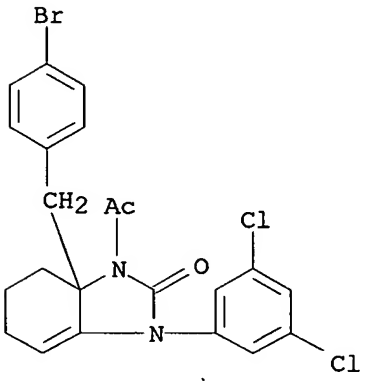
RN 681261-17-6 CAPLUS
CN 2H-Benzimidazol-2-one, 3a-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro-3-methyl- (9CI) (CA INDEX NAME)



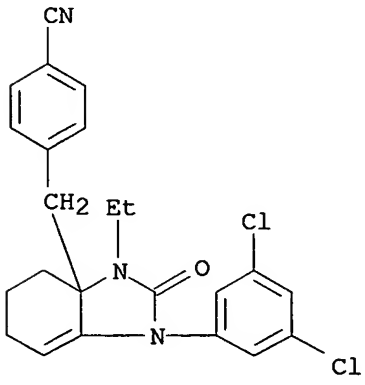
RN 681261-18-7 CAPLUS
CN 2H-Benzimidazol-2-one, 3-acetyl-3a-[(4-cyanophenyl)methyl]-1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro- (9CI) (CA INDEX NAME)



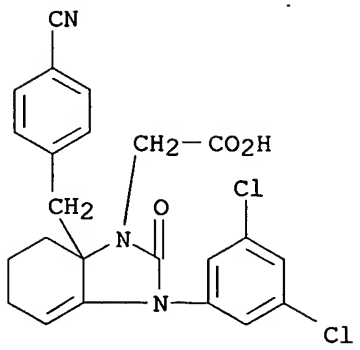
RN 681261-19-8 CAPLUS
CN 2H-Benzimidazol-2-one, 3-acetyl-3a-[(4-bromophenyl)methyl]-1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro- (9CI) (CA INDEX NAME)



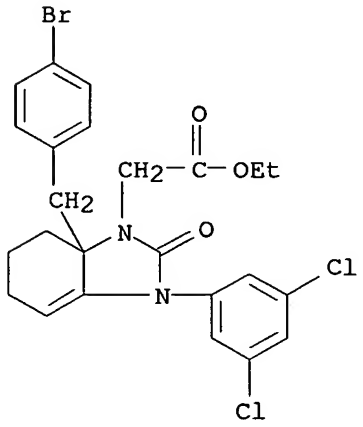
RN 681261-20-1 CAPLUS
CN Benzonitrile, 4-[[1-(3,5-dichlorophenyl)-3-ethyl-1,2,3,4,5,6-hexahydro-2-oxo-3aH-benzimidazol-3a-yl]methyl]- (9CI) (CA INDEX NAME)



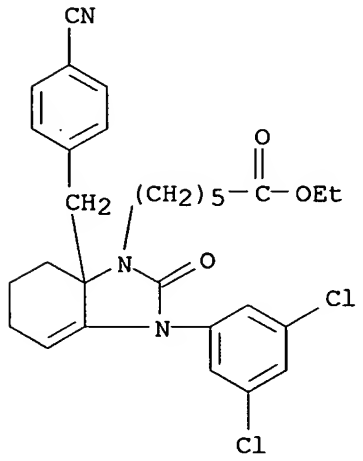
RN 681261-22-3 CAPLUS
CN 1H-Benzimidazole-1-acetic acid, 7a-[(4-cyanophenyl)methyl]-3-(3,5-dichlorophenyl)-2,3,5,6,7,7a-hexahydro-2-oxo- (9CI) (CA INDEX NAME)



RN 681261-23-4 CAPLUS
CN 1H-Benzimidazole-1-acetic acid, 7a-[(4-bromophenyl)methyl]-3-(3,5-dichlorophenyl)-2,3,5,6,7,7a-hexahydro-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)

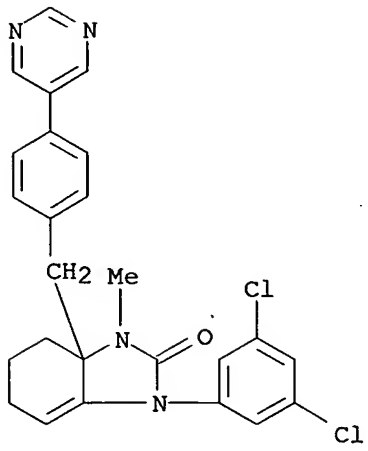


RN 681261-24-5 CAPLUS
CN 1H-Benzimidazole-1-hexanoic acid, 7a-[(4-cyanophenyl)methyl]-3-(3,5-dichlorophenyl)-2,3,5,6,7,7a-hexahydro-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 681261-25-6 CAPLUS

CN 2H-Benzimidazol-2-one, 1-(3,5-dichlorophenyl)-1,3,3a,4,5,6-hexahydro-3-methyl-3a-[[4-(5-pyrimidinyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

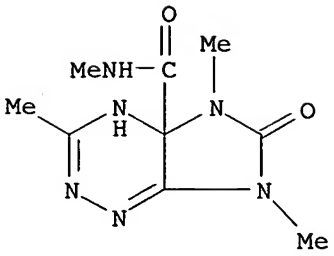


L4 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:499194 CAPLUS
DOCUMENT NUMBER: 125:221409
TITLE: Pyrimidines. XXXIII. Synthesis and properties of new fervenulin derivatives
AUTHOR(S): Werner-Simon, Susanne; Pfleiderer, Wolfgang
CORPORATE SOURCE: Fak. Chem., Univ. Konstanz, Konstanz, D-78434, Germany
SOURCE: Journal of Heterocyclic Chemistry (1996), 33(3), 949-960
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English

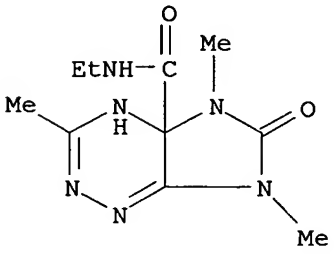
AB A series of new 3-substituted fervenulin (6,8-dimethylpyrimido[5,4-e]-1,2,4-triazine-5,7-dione) derivs. have been synthesized by modifying the 3-alkyl- and aralkyl side-chains. Brominations of 3-methyl-, 3-ethyl- and 3-benzylfervenulin led to mono- and dibromo derivs. which are prone to various nucleophilic displacement reactions. Periodate oxidation and ozonolysis, resp., of 3-styrylfervenulin afforded fervenulin-3-carboxaldehyde which was transformed to a folic acid analog. Potassium permanganate oxidation of 3-alkylfervenulins afforded only ring-contraction to 3-alkyl-5,7-dimethylimidazo[4,5-e]-1,2,4-triazin-6-ones which are also formed as mixts. with their 2,4a-dihydro derivs. on treatment with ethanolic sodium hydroxide. Fervenulin-3-carboxylic acid can be converted to the acid chloride which reacts with amines to fervenulin-3-carboxamides and/or 2,4a-dihydro-5,7-dimethylimidazo[4,5-e]-1,2,4-triazin-6-one-biscarboxamides.

IT **181585-49-9P 181585-51-3P 181585-56-8P**
181585-57-9P 181585-58-0P 181585-59-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fervenulin derivs.)

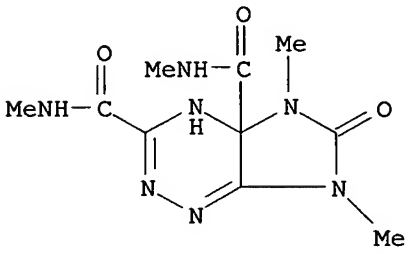
RN 181585-49-9 CAPLUS
CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-4a-carboxamide, 2,5,6,7-tetrahydro-N,3,5,7-tetramethyl-6-oxo- (9CI) (CA INDEX NAME)



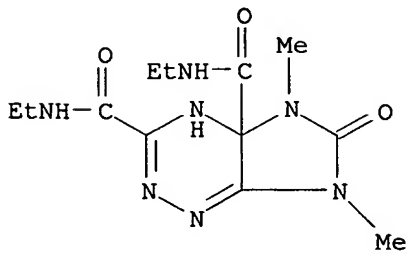
RN 181585-51-3 CAPLUS
CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-4a-carboxamide, N-ethyl-2,5,6,7-tetrahydro-3,5,7-trimethyl-6-oxo- (9CI) (CA INDEX NAME)



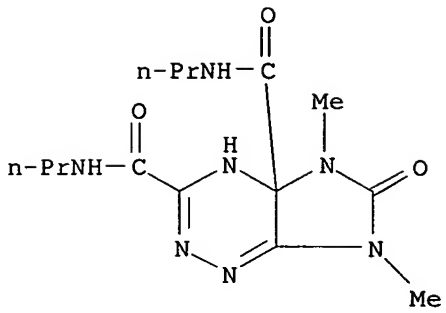
RN 181585-56-8 CAPLUS
CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-3,4a-dicarboxamide, 2,5,6,7-tetrahydro-N,N',5,7-tetramethyl-6-oxo- (9CI) (CA INDEX NAME)



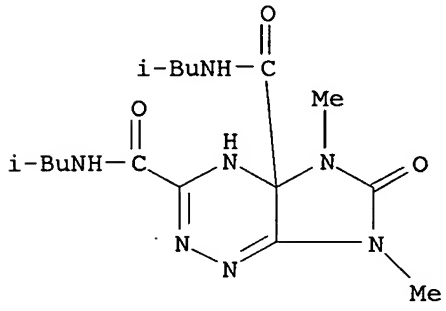
RN 181585-57-9 CAPLUS
CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-3,4a-dicarboxamide, N,N'-diethyl-2,5,6,7-tetrahydro-5,7-dimethyl-6-oxo- (9CI) (CA INDEX NAME)



RN 181585-58-0 CAPLUS
CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-3,4a-dicarboxamide, 2,5,6,7-tetrahydro-5,7-dimethyl-6-oxo-N,N'-dipropyl- (9CI) (CA INDEX NAME)

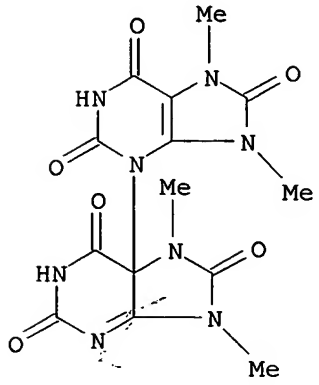


RN 181585-59-1 CAPLUS
CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-3,4a-dicarboxamide, 2,5,6,7-tetrahydro-5,7-dimethyl-N,N'-bis(2-methylpropyl)-6-oxo- (9CI) (CA INDEX NAME)

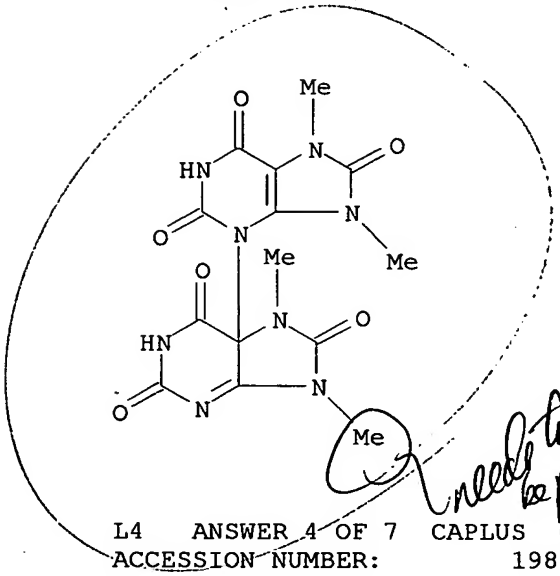


L4 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:430150 CAPLUS
DOCUMENT NUMBER: 111:30150
TITLE: Isolation and characterization of 5-[3'-(7',9'-dimethyluric acid)]-7,9-dimethyl-Δ3,4-isouric acid. An unstable product of electrochemical oxidation of 7,9-dimethyluric acid
AUTHOR(S): Subramanian, P.; Dryhurst, Glenn
CORPORATE SOURCE: Dep. Chem. Biochem., Univ. Oklahoma, Norman, OK, 73019, USA
SOURCE: Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1989), 262(1-2), 281-7
CODEN: JEIEBC; ISSN: 0022-0728
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An account is given of the isolation and structural characterization of the title compound (I) as well as mechanisms for its formation and decomposition
The starting material, 7,9-dimethyluric acid (II), was of com. origin and the electrochem. apparatus was that described earlier. Controlled potential electrooxidn. of II was carried out at 0.65 V in NH4OAc as the supporting electrolyte. To assay the results HPLC, electron impact mass spectrometry, fast-atom bombardment mass spectrometry and similar methods were used.
IT **121263-20-5P 121350-86-5P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of, mechanisms of formation and decomposition in relation to)
RN 121263-20-5 CAPLUS
CN 1H-Purine-2,6,8(3H)-trione, 3-(1,2,6,7,8,9-hexahydro-7,9-dimethyl-2,6,8-

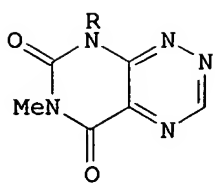
trioxo-5H-purin-5-yl)-7,9-dihydro-7,9-dimethyl-, stereoisomer (9CI) (CA INDEX NAME)



RN 121350-86-5 CAPLUS
CN 1H-Purine-2,6,8(3H)-trione, 3-(1,2,6,7,8,9-hexahydro-7,9-dimethyl-2,6,8-trioxo-5H-purin-5-yl)-7,9-dihydro-7,9-dimethyl-, stereoisomer (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:167430 CAPLUS
DOCUMENT NUMBER: 108:167430
TITLE: Intermediates in the transformation of pyrimido[5,4-e]-1,2,4-triazinediones into imidazo[4,5-e]-1,2,4-triazinones
AUTHOR(S): Shorshnev, S. V.; Esipov, S. E.; Yakushkina, N. I.; Klyuev, N. A.; Zhil'nikov, V. G.; Chernyshev, A. I.
CORPORATE SOURCE: Vses. Nauchno-Issled. Inst. Antibiot., Moscow, 113105, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1987), (9), 1252-9
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 108:167430
GI



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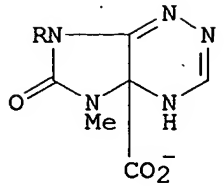

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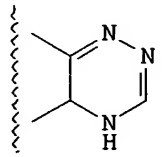

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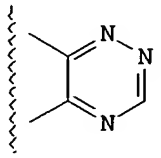


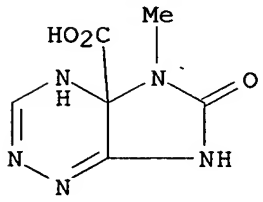
IV

AB Treating pyrimidotriazinediones I (R = H, Me) with aqueous NaOH gave imidazopyrimidinecarboxylic acids II which were decarboxylated by acid to imidazotriazinones III followed by KMnO4 dehydrogenation to give imidazotriazinones IV.

IT **97943-27-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)

RN 97943-27-6 CAPLUS

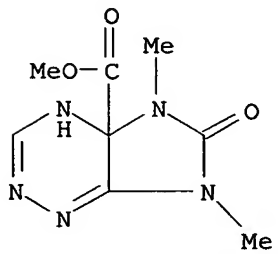
CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-4a-carboxylic acid, 1,2,5,6-tetrahydro-5-methyl-6-oxo- (9CI) (CA INDEX NAME)



IT **113947-23-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 113947-23-2 CAPLUS

CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-4a-carboxylic acid, 2,5,6,7-tetrahydro-5,7-dimethyl-6-oxo-, methyl ester (9CI) (CA INDEX NAME)

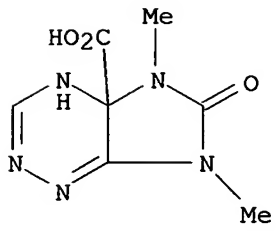


IT **97943-30-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, decarboxylation and esterification of)

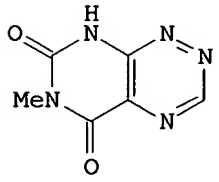
RN 97943-30-1 CAPLUS

CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-4a-carboxylic acid, 2,5,6,7-tetrahydro-

5,7-dimethyl-6-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:156125 CAPLUS
DOCUMENT NUMBER: 106:156125
TITLE: NMR spectroscopic investigation of reumycin alkaline hydrolysis
AUTHOR(S): Shorshnev, S. V.; Esipov, S. E.; Chernyshev, A. I.
CORPORATE SOURCE: All-Union Res. Inst. Antibiot., Moscow, USSR
SOURCE: Antibiotiki i Meditsinskaya Biotekhnologiya (1987), 32(2), 116-20
CODEN: AMBIEH; ISSN: 0233-7525
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



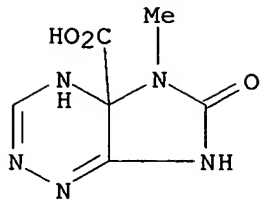
I

AB The transformation sequence of reumycin (I) in aqueous (D2O) solns. with various pD was studied by NMR spectroscopy and the structures of the products were determined Formation of 6-(3-methylureido)-1,2,4-triazine 5-carboxylic acid was the 1st stage of I alkaline hydrolysis. The subsequent cyclization of this compound resulted in the formation of 5-methyl-4,4a-dihydro-5H-imidazo[4,5-e]-1,2,4-triazin-6(7H)one-4a carboxylic acid mono-, di- or trianionic forms depending on the medium pH and due to dissociation of the carboxylic group, N(4)H group of the triazine ring, and N(7)H group of the imidazolidinone ring.

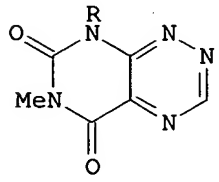
IT **97943-27-6P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in reumycin alkaline hydrolysis)

RN 97943-27-6 CAPLUS

CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-4a-carboxylic acid, 1,2,5,6-tetrahydro-5-methyl-6-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:504756 CAPLUS
DOCUMENT NUMBER: 103:104756
TITLE: Mechanism of conversion of pyrimido[5,4-e]-1,2,4-triazine-5,7-diones to imidazo[4,5-e]-1,2,4-triazin-6-ones in alkaline media
AUTHOR(S): Chernyshev, A. I.; Shorshnev, S. V.; Yakushina, N. I.; Esipov, S. E.
CORPORATE SOURCE: Vses. Nauchno-Issled. Inst. Antibiot., Moscow, 113105, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1985), (2), 277-8
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 103:104756
GI



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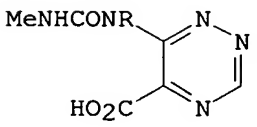

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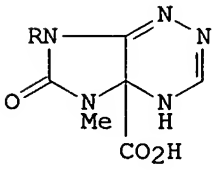

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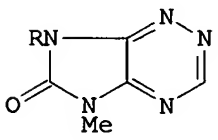


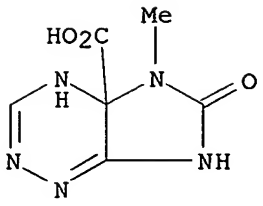
IV

AB Ring cleavage of reumycin (I; R = H) in alkaline solution of pH .apprx.12 gave the triazinecarboxylate II (R = H) which cyclized at pH >13 to give the imidazolotriazinecarboxylate III (R = H). Decarboxylation of the latter and then oxidation by KMnO4 gave the imidazotriazine IV (R = H). Similarly, fervenulin (I; R = Me) was converted to IV (R = Me).

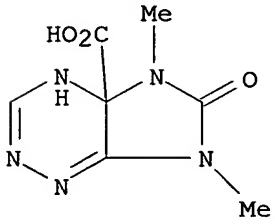
IT **97943-27-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decarboxylation of)

RN 97943-27-6 CAPLUS

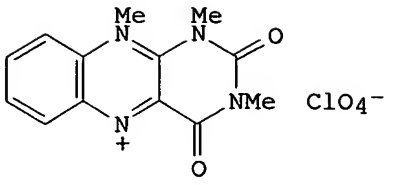
CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-4a-carboxylic acid, 1,2,5,6-tetrahydro-5-methyl-6-oxo- (9CI) (CA INDEX NAME)



IT **97943-30-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 97943-30-1 CAPLUS
CN 4aH-Imidazo[4,5-e]-1,2,4-triazine-4a-carboxylic acid, 2,5,6,7-tetrahydro-5,7-dimethyl-6-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:535265 CAPLUS
DOCUMENT NUMBER: 87:135265
TITLE: Activation and transfer of oxygen. XII. Alkoxy adducts derived from 1,3,10-trimethylalloxazinium (1,3-dimethylflavinium) cations
AUTHOR(S): Mager, H. I. X.
CORPORATE SOURCE: Biochem. Biophys. Lab., Univ. Technol., Delft, Neth.
SOURCE: Tetrahedron (1977), 33(9), 981-9
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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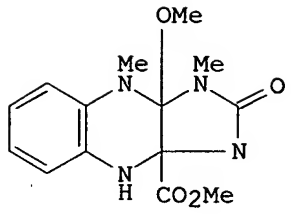

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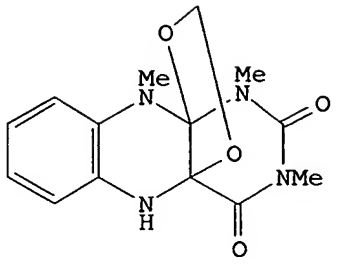


III

AB Alloxazinium cations with alcs. in the presence of base gave monoalkoxy adducts by nucleophilic attack at C-10a. Dialkoxy adducts were formed by subsequent inter- or intramol. nucleophilic attack at C-4 or C-4a. E.g., I with MeOH gave a 4,10a-dialkoxy adduct, by intermol. attack at C-4, which underwent ring contraction to the hexahydroimidazo[4,5-b]quinoxaline II. I with ethylene glycol gave the 4a,10a-ethylenedioxytetrahydroalloxazine III by intramol. attack at C-4a. Thus, the conclusion of V. Massey and P. Hemmerich (1975) and F. Mueller et al. (1976) that the primary addition site is C-9a is in error. Several rearrangements of II were studied.

IT **64270-53-7P**

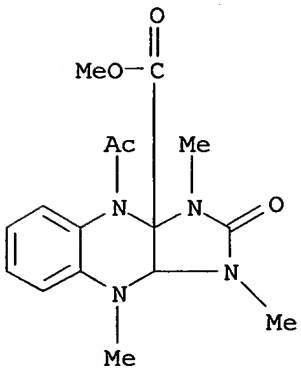
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and heterolysis of)

RN 64270-53-7 CAPLUS

CN 1H-Imidazo[4,5-b]quinoxalinium, 9-acetyl-2,4,9,9a-tetrahydro-9a-(methoxycarbonyl)-1,3,4-trimethyl-2-oxo-, perchlorate (9CI) (CA INDEX NAME)

CM 1

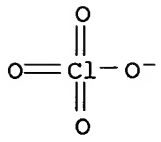
CRN 64270-52-6
CMF C16 H19 N4 O4



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

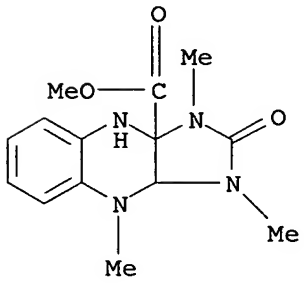
CRN 14797-73-0
CMF Cl O4



IT **64267-62-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, demethoxycarbonylation, rearrangement, and transesterification of)
RN 64267-62-5 CAPLUS
CN 1H-Imidazo[4,5-b]quinoxalinium, 2,4,9,9a-tetrahydro-9a-(methoxycarbonyl)-1,3,4-trimethyl-2-oxo-, perchlorate (9CI) (CA INDEX NAME)

CM 1

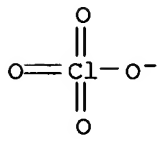
CRN 64267-61-4
CMF C14 H17 N4 O3



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 14797-73-0
CMF Cl O4



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	35.93	197.47

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION

CA SUBSCRIBER PRICE -5.11 -5.11

STN INTERNATIONAL LOGOFF AT 15:06:04 ON 06 APR 2005

Connecting via Winsock to STN

10/681,924

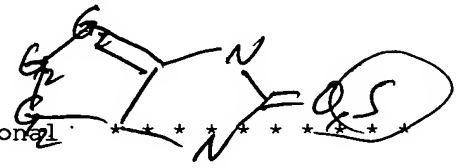
Welcome to STN International! Enter x:x

LOGINID:SSSPTAAJP1626

5-membered rings as ring "1"

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

$G_2 = N, C$



* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	4	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	5	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	6	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	7	MAR 02	GBFULL: New full-text patent database on STN
NEWS	8	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	9	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	10	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	11	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	12	MAR 22	PATDPASPC - New patent database available
NEWS	13	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	14	APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	15	APR 04	EMBASE - Database reloaded and enhanced

NEWS EXPRESS	JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
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FILE 'HOME' ENTERED AT 15:10:25 ON 06 APR 2005

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	0.42

FILE 'REGISTRY' ENTERED AT 15:11:47 ON 06 APR 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2005 HIGHEST RN 847968-12-1
DICTIONARY FILE UPDATES: 5 APR 2005 HIGHEST RN 847968-12-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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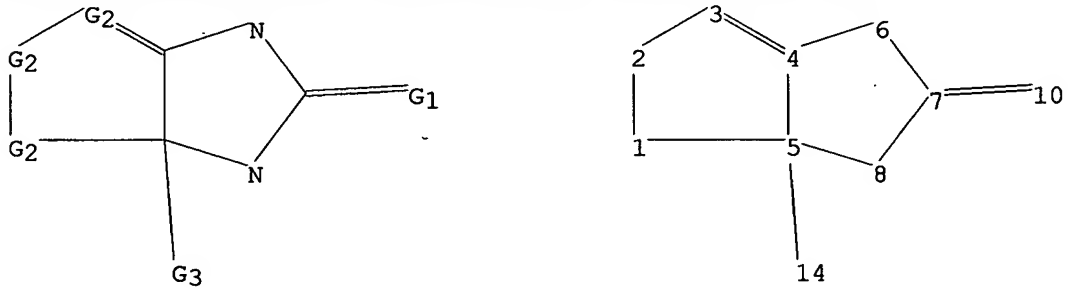

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10 14
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
5-14 7-10
ring bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 7-8
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-14 5-8 6-7 7-8 7-10

G1:O,S

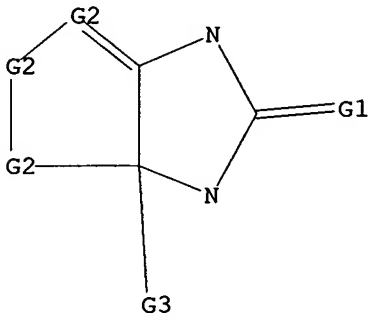
G2:C,N

G3:Cy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS 14:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 O,S

G2 C,N

G3 Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 15:12:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 233513 TO ITERATE

100.0% PROCESSED 233513 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.06

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FILE LAST UPDATED: 5 Apr 2005 (20050405/ED)

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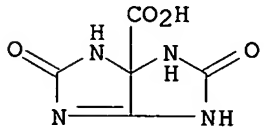
=> s L2
L3 10 L2

=> d L3 1-10 ibib abs hitstr

L3 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:157466 CAPLUS
DOCUMENT NUMBER: 112:157466
TITLE: Kinetics of oxidative ammonolysis of copper(2+) 2,6,8-trioxopurine complex in ammonium buffer
AUTHOR(S): Titskii, G. D.; Miroshnichenko, N. A.
CORPORATE SOURCE: Inst. Phys.-Org. Chem. Coal Chem., Donetsk, USSR
SOURCE: Organic Reactivity (Tartu) (1988), 25(2), 160-9
CODEN: ORREDZ; ISSN: 0131-8314
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The kinetics of oxidizing conversion of Cu2+-2,6,8-trioxypurine complex (I) has been studied spectrophotometrically in ammonium buffer (pH 8.5-10.8) at 25°. The process results from rapid oxidation of I with formation of 1-carboxy-2,4,6,8-tetraaza-3,7-dioxo-4-bicyclo[3.3.0]octene which is bound into Cu2+-NH3 as complex (II). Slow conversion of (II) takes place in two parallel paths.
IT **81129-52-4D**, copper ammonium complexes
RL: PRP (Properties)
(intermediacy of, in oxidative ammonolysis of uric acid complex with cupric ion, kinetics and mechanism and UV in relation to)
RN 81129-52-4 CAPLUS
CN Imidazo[4,5-d]imidazole-3a(1H)-carboxylic acid, 2,3,4,5-tetrahydro-2,5-dioxo- (9CI) (CA INDEX NAME)



L3 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:523129 CAPLUS
DOCUMENT NUMBER: 107:123129
TITLE: Electrochemical oxidation of 9-β-D-ribofuranosyluric acid in basic solution
AUTHOR(S): Tyagi, S. K.; Dryhurst, Glenn
CORPORATE SOURCE: Dep. Chem., Univ. Oklahoma, Norman, OK, 73019, USA
SOURCE: Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1987), 223(1-2), 119-41
CODEN: JEIEBC; ISSN: 0022-0728
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The electrochem. oxidation of 9-β-D-ribofuranosyluric acid (I) was studied at the pyrolytic graphite electrode at pH 9.2. The peak Ia reaction was a 2e--1H+ quasi-reversible process giving an unstable quinonoid which was rapidly attacked by H2O to give 1 and perhaps 2 tertiary alc. intermediates. In the absence of phosphate, these

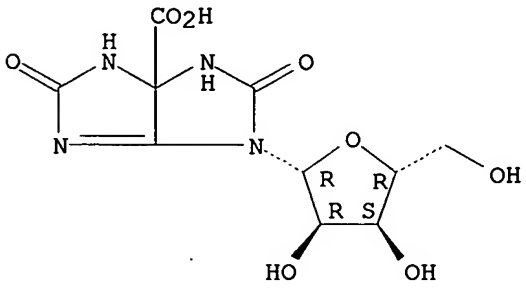
intermediates decompose to give a mixture of 5-hydroxyhydantoin-5-carboxamide-3-riboside, ribose and 4-amino-4-carboxy-2,5-diketo-imidazole. In the presence of phosphate, the putative tertiary alc. intermediate underwent a ring contraction to an electrooxidizable bicyclic carboxylic acid which decomposed to an allantoin riboside. The carboxylic acid was partially responsible for the 2nd, more pos. oxidation peak of I (peak IIa) and in a 2e--1H+ reaction gave 1-hydroxy-2,4,6,8-tetraaza-3,7-dioxo-5-ene-bicyclo(3.3.0)-octane-4-riboside. A stable, peak Ia product also contributed to the peak IIa reaction. This species was a phosphorylated derivative of the bicyclic carboxylic acid. At pH 9.2, in the presence of phosphate, type VIII peroxidase was capable of oxidizing I in a chemical reaction equivalent to the peak Ia electrochem. process.

IT **85303-15-7P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from rearrangement of tertiary alc.)

RN 85303-15-7 CAPLUS

CN Imidazo[4,5-d]imidazole-3a(1H)-carboxylic acid, 2,3,4,5-tetrahydro-2,5-dioxo-1-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:157924 CAPLUS

DOCUMENT NUMBER: 104:157924

TITLE: Electrochemical oxidation of 2,6-diamino-8-purinol

AUTHOR(S): Astwood, D.; D'Amico, C. N.; Lippincott, T.; Brajter-Toth, A.

CORPORATE SOURCE: Dep. Chem., Univ. Maine, Orono, ME, 04469, USA

SOURCE: Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1986), 198(2), 283-302
CODEN: JEIEBC; ISSN: 0022-0728

DOCUMENT TYPE: Journal

LANGUAGE: English

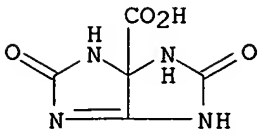
AB Electrochem., spectroelectrochem. and gas chromatog./mass spectrometry were used to determine the mechanism of oxidation of 2,6-diamino-8-purinol [72308-52-2] in phosphate buffer solns. Exptl. evidence indicates that the process is a 2 e-, 2 H+ reaction in which 2,6-diamino-8-purinol is oxidized to form a diimine. The diimine is not stable and decomps. in a series of hydrolysis reactions to the final products 5-hydroxyhydantion-5-carboxamide [36597-25-8] and 3-carbohydroxy-2,4,6,8-tetraza-3,7-dioxo-4-ene-bicyclo[3.3.0]octane. Results are presented which show that the 2 e- oxidation of 2,6-diamino-8-puranol proceeds in two 1 e-1 steps and the evidence for the formation of a coupling product is discussed. A mechanism is proposed to explain the observed results.

IT **81129-52-4P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. oxidation of diaminopurinol in phosphate buffered solution)

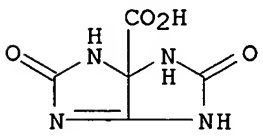
RN 81129-52-4 CAPLUS

CN Imidazo[4,5-d]imidazole-3a(1H)-carboxylic acid, 2,3,4,5-tetrahydro-2,5-

dioxo- (9CI) (CA INDEX NAME)



L3 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:93328 CAPLUS
DOCUMENT NUMBER: 100:93328
TITLE: Electrochemical and enzymatic oxidation of 2,6-diaminopurine
AUTHOR(S): Astwood, D.; Lippincott, T.; Deysher, M.; D'Amico, C.; Szurley, E.; Brajter-Toth, A.
CORPORATE SOURCE: Dep. Chem., Univ. Maine, Orono, ME, 04469, USA
SOURCE: Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1983), 159(2), 295-312
CODEN: JEIEBC; ISSN: 0022-0728
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Electrochem. spectroelectrochem., gas chromatog./mass spectrometry (GC/MS) were used to study the mechanism of electrochem. oxidation of 2,6-diaminopurine [1904-98-9] in aqueous solns. Exptl. evidence indicates that the oxidation pathway depends on potential. At less pos. potentials 2,6-diaminopurine is initially oxidized in a 2 e-,2 H+ reaction to 2,6-diamino-8-purinol [72308-52-2] which is immediately further oxidized to the 2,6-diaminopurinol-diimine in a 2 e-, 2 H+ reaction. At more pos. potentials 4 e and 4 H+ are exchanged to form the diimine. The diimine is not stable and decomps. in a series of hydrolysis reactions to the final products 5-hydroxyhydantoin-5-carboxamide [36597-25-8] and 1-carbohydroxy-2,4,6,8-tetraaza-3,7-dioxo-4-ene-bicyclo[3.3.0]octane [**81129-52-4**]. The products were identified by GC/MS. A mechanism is proposed to explain the observed results. The significance of this mechanism with respect to the enzymic oxidation and deamination of 2,6-diaminopurine is discussed.
IT **81129-52-4P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. oxidation of diaminopurine in aqueous solns.)
RN 81129-52-4 CAPLUS
CN Imidazo[4,5-d]imidazole-3a(1H)-carboxylic acid, 2,3,4,5-tetrahydro-2,5-dioxo- (9CI) (CA INDEX NAME)



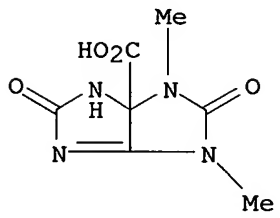
L3 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:620927 CAPLUS
DOCUMENT NUMBER: 99:220927
TITLE: Electrochemical oxidation of 7,9-dimethyluric acid in acid solution
AUTHOR(S): Chen, Tsuyu Raymond; Dryhurst, Glenn
CORPORATE SOURCE: Dep. Chem., Univ. Oklahoma, Norman, OK, 73019, USA
SOURCE: Journal of Electroanalytical Chemistry and Interfacial

Electrochemistry (1983), 154(1-2), 107-19
CODEN: JEIEBC; ISSN: 0022-0728
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The electrochem. oxidation of 7,9-dimethyluric acid [19039-41-9] at pH 3-5 was studied by using a pyrolytic graphite electrode. Two voltammetric oxidation peaks (Ia and IIa) were observed Peak Ia is a 2e--1H+ reaction yielding a very reactive quinoid cation that, in a reaction catalyzed by H2PO4-, is hydrated to an UV-absorbing tertiary alc. intermediate. This intermediate can undergo ring contraction to give 1-carboxy-2,4-dimethyl-2,4,6,8-tetraaza-3,7-dioxo-5-ene-bicyclo[3.3.0]octane (I) [**85303-22-6**] or react with H2PO4- and 7,9-dimethyluric acid to give a relatively long-lived complex. The I is hydrated and decomps. to 1,3-dimethylallantoin [32282-45-4]. The tertiary alc.-H2PO4--7,9-dimethyluric acid complex very slowly decomps. regenerating 7,9-dimethyluric acid and, ultimately, 1,3-dimethyl-5-hydroxyhydan-5-carboxamide [87897-69-6]. Peak IIa is a minor process and is due to 2e- oxidation of the anion of I in a Kolbe-type reaction giving 1-hydroxy-2,4-dimethyl-2,4,6,8-tetraaza-3,7-dioxo-5-ene-bicyclo[3.3.0]octane [85303-23-7].

IT **85303-22-6P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. oxidation of dimethyluric acid in acid phosphate buffer solution)

RN 85303-22-6 CAPLUS
CN Imidazo[4,5-d]imidazole-3a(1H)-carboxylic acid, 2,3,4,5-tetrahydro-1,3-dimethyl-2,5-dioxo- (9CI) (CA INDEX NAME)



L3 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:169134 CAPLUS
DOCUMENT NUMBER: 98:169134
TITLE: The electrochemical and peroxidase-catalyzed redox chemistry of 9-β-D-ribofuranosyluric acid
AUTHOR(S): Goyal, R. N.; Brajter-Toth, Anna; Besca, Joseph S.; Dryhurst, Glenn
CORPORATE SOURCE: Dep. Chem., Univ. Oklahoma, Norman, OK, 73019, USA
SOURCE: Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1983), 144(1-2), 163-90
CODEN: JEIEBC; ISSN: 0022-0728
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The electrochem. oxidation of 9-β-D-ribofuranosyluric acid (I) [21082-30-4] at a pyrolytic graphite electrode proceeds via an initial 2 e- reaction to give an unstable quinonoid intermediate. Nucleophilic attack by water of this intermediate leads to isomeric tertiary alc. intermediates. The latter were characterized by electrochem. reduction to a dihydro product which readily dehydrates to regenerate I. The tertiary alc. intermediates can undergo a ring-opening reaction at pH ≥ 6 to give a spectrally distinct and reversibly reducible pyrimidine derivative(s) which slowly decompose to give alloxan or alloxanic acid and urea riboside. Alternatively, the tertiary alc. can further hydrate to yield, ultimately,

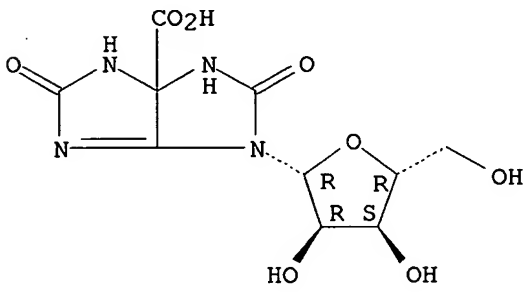
5-hydroxyhydrantoin-5-carboxamide-3-riboside [85303-13-5] or undergo a ring contraction reaction and hydrolysis leading to allantoin riboside [85303-14-6]. The peroxidase-catalyzed oxidation appears to follow essentially the same chemical pathway.

IT **85303-15-7P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. oxidation of ribofuranosyluric acid)

RN 85303-15-7 CAPLUS

CN Imidazo[4,5-d]imidazole-3a(1H)-carboxylic acid, 2,3,4,5-tetrahydro-2,5-dioxo-1-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1983:151660 CAPLUS

DOCUMENT NUMBER: 98:151660

TITLE: The second voltammetric oxidation peak of 7,9-dimethyluric acid

AUTHOR(S): Chen, Tsuyu Raymond; Dryhurst, Glenn

CORPORATE SOURCE: Dep. Chem., Univ. Oklahoma, Norman, OK, 73019, USA

SOURCE: Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1983), 144(1-2), 191-206
CODEN: JEIEBC; ISSN: 0022-0728

DOCUMENT TYPE: Journal

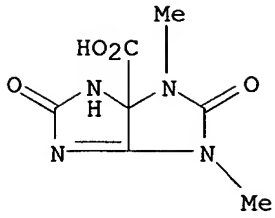
LANGUAGE: English

AB Voltammetry of 7,9-dimethyluric acid [19039-41-9] in aqueous solution at a pyrolytic graphite electrode shows that 2 oxidation peaks are formed. Peak Ia is a 2-e electrooxidn. giving a very unstable quinonoid cation. This rapidly hydrates in a phosphate-catalyzed reaction giving a tertiary alc., which in turn undergoes a ring contraction to 1-carbohydroxy-2,4-dimethyl-2,4,6,8-tetraaza-3,7-dioxo-5-enebicyclo[3.3.0]octane [**85303-22-6**]. The latter is again unstable and hydrates and decarboxylates, giving 1,3-dimethylallantoin [32282-45-4] as the final product. Peak IIa is due to a Kolbe-type 2-e electrooxidn. of 1-carbohydroxy-2,4-dimethyl-2,4,6,8-tetraaza-3,7-dioxo-5-enebicyclo[3.3.0]octane to give a very reactive carbonium ion and CO2. The former species is rapidly hydrated, giving 1-hydroxy-2,4-dimethyl-2,4,6,8-tetraaza-3,7-dioxo-5-enebicyclo[3.3.0]octane [85303-23-7], a new compound which has been isolated and characterized by spectral, chemical and electrochem. methods.

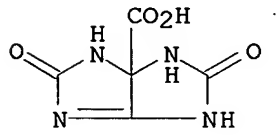
IT **85303-22-6**
RL: PRP (Properties)
(electrochem. oxidation of electrogenerated intermediate of, in dimethyluric acid electrochem. oxidation)

RN 85303-22-6 CAPLUS

CN Imidazo[4,5-d]imidazole-3a(1H)-carboxylic acid, 2,3,4,5-tetrahydro-1,3-dimethyl-2,5-dioxo- (9CI) (CA INDEX NAME)



L3 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:571170 CAPLUS
DOCUMENT NUMBER: 97:171170
TITLE: Spectroelectrochemical evidence for imine-alcohol intermediate formed upon electrochemical oxidation of uric acid
AUTHOR(S): Goyal, R. N.; Nguyen, N. T.; Dryhurst, Glenn
CORPORATE SOURCE: Dep. Chem., Univ. Oklahoma, Norman, OK, 73019, USA
SOURCE: Bioelectrochemistry and Bioenergetics (1982), 9(3), 273-85
CODEN: BEBEBP; ISSN: 0302-4598
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Electrochem. oxidation of uric acid [69-93-2] in phosphate-containing supporting electrolytes at pH 3-9 at a reticulated vitreous C electrode in a thin-layer spectroelectrochem. cell leads to formation of UV-absorbing intermediate species. Electrochem. reduction of the intermediate-containing solution leads to the partial regeneration of uric acid. This behavior provides compelling evidence that an imine-alc. is 1 of the UV-absorbing intermediate species because only this compound may be expected to be reduced to a species which can regenerate uric acid.
IT **81129-52-4**
RL: PRP (Properties)
(intermediate, in uric acid electrochem. oxidation)
RN 81129-52-4 CAPLUS
CN Imidazo[4,5-d]imidazole-3a(1H)-carboxylic acid, 2,3,4,5-tetrahydro-2,5-dioxo- (9CI) (CA INDEX NAME)



L3 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:467958 CAPLUS
DOCUMENT NUMBER: 97:67958
TITLE: A comparison of the peroxidase-catalyzed and electrochemical oxidation of uric acid
AUTHOR(S): Goyal, R. N.; Brajter-Toth, Anna; Dryhurst, Glenn; Nguyen, N. T.
CORPORATE SOURCE: Dep. Chem., Univ. Oklahoma, Norman, OK, 73019, USA
SOURCE: Bioelectrochemistry and Bioenergetics (1982), 9(1), 39-60
CODEN: BEBEBP; ISSN: 0302-4598
DOCUMENT TYPE: Journal

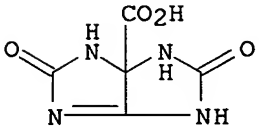
LANGUAGE: English

AB The oxidation of uric acid by H2O2 in the presence of type VIII peroxidase was studied between pH 5.2 and 8. Intermediates generated in the reaction were characterized in terms of their UV spectra and kinetics of decay. In addition ≥1 UV-absorbing intermediate was trapped, converted to its trimethylsilyl derivative, and identified by gas chromatog.-mass spectrometry. This intermediate is 1-carbohydroxy-2,4,6,8-tetraza-3,7-dioxo-4-ene-bicyclo-(3.3.0)-octane. At pH ≥7 the product is allantoin, whereas at lower pH 5-hydroxyhydantoin-5-carboxamide is also formed as a major product. The intermediates and products formed and spectral and kinetic measurements observed during and after peroxidase-catalyzed oxidation of uric acid are virtually identical to those noted upon electrochem. oxidation Thus, the mechanisms of electrochem. and enzymic oxidation of uric acid are, in a chemical sense, identical.

IT **81129-52-4**
RL: BIOL (Biological study)
(as urate peroxidase-catalyzed oxidation intermediate)

RN 81129-52-4 CAPLUS

CN Imidazo[4,5-d]imidazole-3a(1H)-carboxylic acid, 2,3,4,5-tetrahydro-2,5-dioxo- (9CI) (CA INDEX NAME)



L3 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1982:151261 CAPLUS

DOCUMENT NUMBER: 96:151261

TITLE: Further insights into the electrochemical oxidation of uric acid

AUTHOR(S): Goyal, R. N.; Brajter-Toth, Anna; Dryhurst, Glenn

CORPORATE SOURCE: Dep. Chem., Univ. Oklahoma, Norman, OK, 73019, USA

SOURCE: Journal of Electroanalytical Chemistry and Interfacial Electrochemistry (1982), 131, 181-202
CODEN: JEIEBC; ISSN: 0022-0728

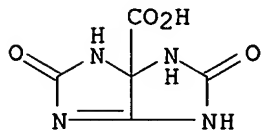
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The electrochem. oxidation of uric acid [69-93-2] was studied between pH 1.5 and 9.5 in phosphate buffers using thin-layer spectroelectrochem. to generate and study UV-absorbing intermediates. It was concluded, on the basis of this and preceding studies, that uric acid is 1st oxidized in a 2e--2H+ reaction to a very unstable quinonoid diimine(half-life ≤ 22 ms). At pH ≥ 6 the anion of the latter species is attacked by water to give an anionic imine-alc. that undergoes a ring contraction reaction to give 1-carbohydroxy-2,4,6,8-tetraaza-3,7-dioxo-4-enebicyclo[3.3.0]octane [**81129-52-4**]. This then decomps. to allantoin [97-59-6]. At pH 3-5.6 a neutral quinonoid diimine is generated upon 2e--2H+ oxidation of uric acid. In high-phosphate buffers H2PO4- attacks the diimine, whereas in low-phosphate buffers solvent (H2O) attacks the diimine. In high-phosphate buffers anal. of absorbance vs. time curves obtained following oxidation of uric acid in a thin-layer cell allows 3 intermediate species to be inferred. In low-phosphate buffers only 2 intermediates may be inferred. Mechanisms are advanced to rationalize these observations and to account for the end products formed., i.e. allantoin, 5-hydroxyhydantoin-5-carboxamide [36597-25-8] and, at pH 3, alloxan [50-71-5].

IT **81129-52-4P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, in electrochem. oxidation of uric acid in phosphate-buffered solution)
RN 81129-52-4 CAPLUS
CN Imidazo[4,5-d]imidazole-3a(1H)-carboxylic acid, 2,3,4,5-tetrahydro-2,5-dioxo- (9CI) (CA INDEX NAME)



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FULL ESTIMATED COST	51.20	212.95

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-7.30	-7.30

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DICTIONARY FILE UPDATES: 5 APR 2005 HIGHEST RN 847968-12-1

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